WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

identifying a test compound that modulates coactivator binding to said nuclear receptor.

2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.

3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

8. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

Sub A3 9. The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

10. The method of claim 1, wherein said screening is *in vitro*.

11. The method of claim 10, wherein said screening is high throughput screening.

Sub B3 12. The method of claim 1, wherein said assay is a biological assay.

13. The method of claim 1, wherein said test compound is from a library of compounds.

14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.

Sub C4 15. The method of ~~claim 14~~, wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.

Sub A4 16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.

17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

19. The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.

20. The machine readable storage medium of claim 19, wherein said thyroid receptor is human.

21. The machine readable storage medium of claim 20, wherein said molecule is peptide.

22. The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.

23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

24. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of

machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.

26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.

27. The cocrystal of claim 26, wherein said thyroid receptor is human.

28. The cocrystal of claim 27, wherein said molecule is peptide.

29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.

30. A compound identified according to the method of claim 1.

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